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Abstract

In a probabilistic cellular automaton (PCA), the cells are updated synchronously and independently, according to a distribution depending on a finite neighborhood. A PCA can be viewed as a Markov chain whose ergodicity is investigated. A classical cellular automaton (CA) is a particular case of PCA. For a 1-dimensional CA, we prove that ergodicity is equivalent to nilpotency, and is therefore undecidable. We then propose an efficient perfect sampling algorithm for the invariant measure of an ergodic PCA. Our algorithm does not assume any monotonicity property of the local rule. It is based on a bounding process which is shown to be also a PCA.

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1 Introduction

Cellular automata (CA) are dynamical systems in which space and time are discrete. A cellular automaton consists of a lattice (e.g. $\mathbb{Z}^d$ or $\mathbb{Z}/n\mathbb{Z}$) divided in regular cells, each cell containing a letter of a finite alphabet. The cells evolve synchronously, each one evolving in function of a finite number of cells in its neighborhood, according to a local rule.

To take into account randomness, one is led to consider *probabilistic cellular automata* (PCA) [17]. For PCA, time is dicrete and the cells evolve synchronously as for CA, but the difference is that for each cell, the new content is randomly chosen, independently of the others, according to a distribution depending only on a finite neighborhood of the cell.

Let us mention a couple of motivations. First, the investigation of fault-tolerant computational models was the motivation for the russian school to study PCA [17, 6]. Second, PCA appear in combinatorial problems related to the enumeration of directed animals [11]. Third, in the context of the classication of CA (Wolfram's program), robustness to random errors can be used as a discriminating criterion [5, 14].

We focus our study on the equilibrium behavior of PCA. Observe that a PCA may be viewed as a Markov chain over the state space $\mathcal{A}^E$, where $\mathcal{A}$ is the alphabet and E is the set of cells. The equilibrium is studied via the invariant measures of the Markov chain. A PCA is *ergodic* if it has a unique and attractive invariant measure. Finding conditions to ensure ergodicity is a difficult problem which has been thoroughly investigated [17, 6]. When a PCA is ergodic, it is usually impossible to determine the invariant measure explicitly, and

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simulation becomes the alternative. Simulating PCA is known to be a challenging task, costly both in time and space. Also, configurations cannot be tracked down one by one (there is an infinite number of them when E is infinite) and may only be observed through some measured parameters. The point is to have guarantees upon the results obtained from simulations.

In this context, our contributions are as follows. First, we prove that the ergodicity of a CA on $\mathbb{Z}$ is undecidable. This was mentioned as *Unsolved Problem 4.5* in [16]. Since a CA is a special case of a PCA, it also provides a new proof of the undecidability of the ergodicity of a PCA (Kurdyumov, see [17, Chap. 14], and Toom [15]). Second, we propose an efficient perfect sampling algorithm for ergodic PCA. Recall that a *perfect sampling* procedure is a random algorithm which returns a configuration distributed according to the invariant measure. By applying the procedure repeatedly, we can estimate the invariant measure with arbitrary precision. We propose such an algorithm for PCA by adapting the *coupling from the past* method of Propp & Wilson [12]. When the set of cells is finite, a PCA is a finite state space Markov chain. Therefore, coupling from the past from all possible initial configurations provides a basic perfect sampling procedure, but a very inefficient one since the number of configurations is exponential in the number of cells. Here, the contribution consists in an important simplification of the procedure. We define a new PCA on an extended alphabet, called the *envelope PCA* (EPCA). We obtain a perfect sampling procedure for the original PCA by running the EPCA on a single initial configuration. When the set of cells is infinite, a PCA is a Markov chain on an uncountable state space. So there is no basic perfect sampling procedure anymore. We prove the following: If the PCA is ergodic, then the EPCA may or may not be ergodic. If it is ergodic, then we can use the EPCA to design an efficient perfect sampling procedure (the result of the algorithm is the finite restriction of a configuration with the right invariant distribution). The EPCA can be viewed as a systematic treatment of ideas already used by Toom for *percolation PCA* (see for instance [16, Section 2]).

The perfect sampling procedure can also be run on a PCA whose ergodicity is unknown, with the purpose of testing it. We illustrate this approach on *Majority*, prototype of a PCA whose equilibrium behavior is not well understood.

2 Probabilistic cellular automata

Let $\mathcal{A}$ be a finite set called the *alphabet*, and let E be a countable or finite set of *cells*. We denote by X the set $\mathcal{A}^E$ of *configurations*.

We assume that E is equipped with a commutative semigroup structure, whose law is denoted by $+$. In examples, we consider mostly the cases $E = \mathbb{Z}$ or $E = \mathbb{Z}/n\mathbb{Z}$. Given $K \subset E$ and $V \subset E$, we define $V + K = \{v + k \mid v \in V, k \in K\}$.

A *cylinder* is a subset of X having the form $\{x \in X \mid \forall k \in K, x_k = y_k\}$ for a given finite subset K of E and a given element $(y_k)_{k\in K} \in \mathcal{A}^K$. When there is no possible confusion, we shall denote briefly by y_K the cylinder $\{x \in X \mid \forall k \in K, x_k = y_k\}$. For a given finite subset K, we denote by $\mathcal{C}(K)$ the set of all cylinders of base K.

Let us equip $X = \mathcal{A}^E$ with the product topology, which can be described as the topology generated by cylinders. We denote by $\mathcal{M}(\mathcal{A})$ the set of probability measures on $\mathcal{A}$ and by $\mathcal{M}(X)$ the set of probability measures on X for the σ-algebra generated by all cylinder sets, which corresponds to the Borelian σ-algebra. For $x \in X$, denote by δ_x the Dirac measure concentrated on the configuration x.

▶ **Definition 2.1.** Given a finite set $V \subset E$, a *transition function* of *neighborhood* V is a function $f : \mathcal{A}^V \to \mathcal{M}(\mathcal{A})$. The *probabilistic cellular automaton* (PCA) P of transition

function f is the application $P : \mathcal{M}(X) \to \mathcal{M}(X),\ \mu \mapsto \mu P$, defined on cylinders by:

$$\mu P(y_K) = \sum_{x_{V+K} \in \mathcal{C}(V+K)} \mu(x_{V+K}) \prod_{k \in K} f((x_{k+v})_{v \in V})(y_k)\,.$$

Let us look at how P acts on a Dirac measure δ_z. The content z_k of the k-th cell is changed into the letter $a \in \mathcal{A}$ with probability $f((z_{k+v})_{v\in V})(a)$, independently of the evolution of the other cells. The real number $f((z_{k+v})_{v\in V})(a) \in [0,1]$ is thus to be thought as the conditional probability that, after application of P, the k-th cell will be in the state a if, before its application, the neighborhood of k was in the state $(z_{k+v})_{v\in V}$.

Let u be the uniform measure on $[0,1]$. We define the product measure $\tau = \bigotimes_{i\in E} u$ on $[0,1]^E$.

▶ **Definition 2.2.** An *update function* of the probabilistic cellular automaton P is a deterministic function $\phi : \mathcal{A}^E \times [0,1]^E \to \mathcal{A}^E$ (the function ϕ takes as argument a configuration and a sample in $[0,1]^E$, and returns a new configuration), satisfying for each $x \in \mathcal{A}^E$, and each cylinder y_K,

$$\tau(\{r \in [0,1]^E; \phi(x,r) \in y_K\}) = \prod_{k\in K} f((x_{k+v})_{v\in V})(y_k).$$

In practice, it is always possible to define an update function ϕ for which the value of $\phi(x,r)_k$ only depends on $(x_{k+v})_{v\in V}$ and on r_k. For example, if the alphabet is $\mathcal{A} = \{a_1, \dots, a_n\}$, one can set

$$\phi(x,r)_k = \begin{cases} a_1 & \text{if } \ 0 \le r_k < f((x_{k+v})_{v\in V})(a_1) \\ a_2 & \text{if } \ f((x_{k+v})_{v\in V})(a_1) \le r_k < f((x_{k+v})_{v\in V})(\{a_1,a_2\}) \\ \vdots & \\ a_n & \text{if } \ f((x_{k+v})_{v\in V}(\{a_1,a_2,\dots,a_{n-1}\}) \le r_k \le 1. \end{cases} \tag{1}$$

For a given initial configuration $x^0 \in \mathcal{A}^E$, and samples $(r^t)_{t\in\mathbb{N}},\ r^t \in [0,1]^E$, let $(x^t)_{t\in\mathbb{N}} \in (\mathcal{A}^E)^{\mathbb{N}}$ be the sequence defined recursively by $x^{t+1} = \phi(x^t, r^t)$. Such a sequence is called a *space-time diagram*. It can be viewed as a realization of the Markov chain. Examples of space-time diagrams appear in Figures 1 and 2.

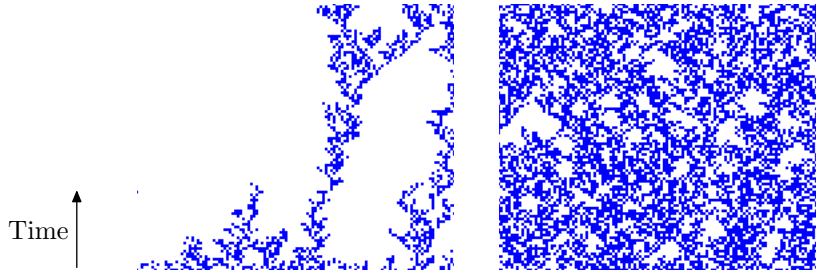
Classical cellular automata are a specialization of PCA.

▶ **Definition 2.3.** A *deterministic cellular automaton* (DCA) is a PCA such that for each sequence $(x_v)_{v\in V} \in \mathcal{A}^V$, the measure $f((x_v)_{v\in V})$ is concentrated on a single letter of the alphabet. A DCA can thus be seen as a deterministic function $F : \mathcal{A}^E \to \mathcal{A}^E$.

In the literature, the term *cellular automaton* denotes what we call here a DCA. Deterministic cellular automata have been widely studied, in particular on the set of cells $E = \mathbb{Z}$, see Section 3. For a DCA, any initial configuration defines a unique space-time diagram.

▶ **Example 2.4.** Let $\mathcal{A} = \{0,1\}$, $E = \mathbb{Z}$, and $V = \{0,1\}$. Consider $0 < \varepsilon < 1$ and the local function $f(x,y) = (1-\varepsilon)\,\delta_{x+y \mod 2} + \varepsilon\,\delta_{x+y+1 \mod 2}$. This defines a PCA that can be considered as a perturbation of the DCA $F : \mathcal{A}^E \to \mathcal{A}^E$ defined by $F(x)_i = x_i + x_{i+1} \mod 2$, with errors occuring in each cell independently with probability ε.

▶ **Example 2.5.** Let $\mathcal{A} = \{0,1\}$, $E = \mathbb{Z}^d$, and let V be a finite subset of E. Consider $0 < \alpha < 1$ and the local function: $f((x_v)_{v\in V}) = \alpha\,\delta_{\max(x_v,\ v\in V)} + (1-\alpha)\,\delta_0$. The corresponding PCA is called the *percolation PCA* associated with V and α. The particular case of the space $E = \mathbb{Z}$ and the neighborhood $V = \{0,1\}$ is called the *Stavskaya PCA*. In Figure 1, we represent two portions of diagrams of the percolation PCA for $E = \mathbb{Z}$ and $V = \{-1,0,1\}$.



(a) $\alpha = 0.5$ **(b)** $\alpha = 0.6$

Figure 1 Space-time diagrams of the PCA of Example 2.5, for $V = \{-1, 0, 1\}$.

2.1 Invariant measures and ergodicity

A PCA can be seen as a Markov chain on the state space $\mathcal{A}^E$. We use the classical terminology for Markov chains that we now recall.

▶ **Definition 2.6.** A probability measure $\pi \in \mathcal{M}(X)$ is said to be an *invariant measure* of the PCA P if $\pi P = \pi$. The PCA is *ergodic* if it has exactly one invariant measure π which is *attractive*, that is, for any measure $\mu \in \mathcal{M}(X)$, the sequence μP^n converges weakly to π (*i.e.* for any cylinder C, $\lim_{n\to+\infty} \mu P^n(C) = \pi(C)$).

A PCA has at least one invariant measure, and the set of invariant measures is convex and compact. This is a standard fact, based on the observation that the set $\mathcal{M}(X)$ of measures on X is compact for the weak topology, see for instance [17]. Therefore, there are three possible situations for a PCA:

(*i*) several invariant measures; (*ii*) a unique invariant measure which is not attractive; (*iii*) a unique invariant measure which is attractive (ergodic case).

▶ **Example 2.7.** Consider the PCA of Example 2.4. Using the results in [17, Chapters 16 and 17], one can prove that the PCA is ergodic and that its unique invariant measure is the uniform mesure, *i.e.* the product of Bernoulli measures of parameter 1/2.

▶ **Example 2.8.** Consider the percolation PCA of Example 2.5. Observe that the Dirac measure δ_{0^E} is an invariant measure. Using a coupling with a percolation model, one can prove the following, see for instance [16, Section 2]. There exists $\alpha^* \in (0, 1)$ such that:

$\alpha < \alpha^* \implies (iii)$: ergodicity, $\alpha > \alpha^* \implies (i)$: several invariant measures.

The exact value of α^* is not known but it satisfies $1/|V| \leq \alpha^* \leq 53/54$.

The existence of a PCA corresponding to situation (*ii*) had been a long standing conjecture, but an example has recently been presented in [3]. The PCA of Example 2.5 exhibits a phase transition between the situations (*i*) and (*iii*). In Section 5, we study a PCA that may have a phase transition between the situations (*ii*) and (*iii*). It would provide the first example of this type.

3 Ergodicity of DCA

DCA form the simplest class of PCA, it is therefore natural to study the ergodicity of DCA. In this section, we prove the undecidability of ergodicity for DCA (Theorem 3.4).

Remark. In the context of DCA, the terminology of Definition 2.6 might be confusing. Indeed a DCA P can be viewed in two different ways: (*i*) a (degenerated) Markov chain;

(*ii*) a symbolic dynamical system. In the dynamical system terminology, P is *uniquely ergodic* if: $[\exists!\mu,\ \mu P = \mu]$. In the Markov chain terminology (that we adopt), P is *ergodic* if: $[\exists!\mu,\ \mu P = \mu]$ and $[\forall\nu,\ \nu P^n \xrightarrow{w} \mu]$, where $\xrightarrow{w}$ stands for the weak convergence. Knowing if the unique ergodicity (of symbolic dynamics) implies the ergodicity (of the Markov theory) is an open question for DCA.

The *limit set* of P is defined by $LS = \bigcap_{n\in\mathbb{N}} P^n(\mathcal{A}^E)$. In words, a configuration belongs to LS if it may occur after an arbitrarily long evolution of the cellular automaton. Observe that LS is non-empty since it is the decreasing limit of non-empty closed sets. A constructive way to show that LS is non-empty is as follows. The image by P of a monochromatic configuration x^E is monochromatic: $x^E \to y^E$. In particular, there exists a monochromatic periodic orbit for P, and we have: $x_0^E \to x_1^E \to \cdots \to x_{k-1}^E \to x_0^E \implies \{x_0^E, x_1^E, \ldots, x_{k-1}^E\} \subset LS$.

Recall that δ_u denotes the probability measure concentrated on the configuration u. The periodic orbit $(x_0^E, \ldots, x_{k-1}^E)$ provides an invariant measure given by $(\delta_{x_0^E} + \ldots + \delta_{x_{k-1}^E})/k$. More generally, the support of any invariant measure is included in the limit set.

▶ **Definition 3.1.** A DCA is *nilpotent* if its limit set is a singleton.

Clearly, a DCA is nilpotent iff $LS = \{x^E\}$ for some $x \in \mathcal{A}$. The following stronger statement is proved in [4], using a compactness argument:

$$[\ P \text{ nilpotent}\ ] \iff [\ \exists x \in \mathcal{A}, \exists N \in \mathbb{N},\ \ P^N(\mathcal{A}^E) = \{x^E\}\ ]\,.$$

In that case, for any probability measure μ on $\mathcal{A}^E$, we have $\mu P^N = \delta_{x^E}$, so that P is ergodic with unique invariant measure δ_{x^E}. This proves the following proposition.

▶ **Proposition 3.2.** *Consider a DCA P. We have:* $[\ P \text{ nilpotent}\ ] \implies [\ P \text{ ergodic}\ ]$.

If we restrict ourselves to DCA on $\mathbb{Z}$, we get the converse statement.

▶ **Theorem 3.3.** *Consider a DCA P on the set of cells $\mathbb{Z}$. We have:*

$$[\ P \text{ nilpotent}\ ] \iff [\ P \text{ ergodic}\ ]\,.$$

Proof. Let P be an ergodic DCA. Assume that there exists a monochromatic periodic orbit $(x_0^{\mathbb{Z}}, \ldots, x_{k-1}^{\mathbb{Z}})$ with $k \geq 2$. Then $\mu = (\delta_{x_0^{\mathbb{Z}}} + \cdots + \delta_{x_{k-1}^{\mathbb{Z}}})/k$ is the unique invariant measure. The sequence $\delta_{x_0^{\mathbb{Z}}} P^n$ does not converge weakly to μ, which is a contradiction. Therefore, there exists a monochromatic fixed point: $P(x^{\mathbb{Z}}) = x^{\mathbb{Z}}$, and $\delta_{x^{\mathbb{Z}}}$ is the unique invariant measure.

Define the cylinder $C = \{v \in \mathcal{A}^{\mathbb{Z}} \mid \forall i \in K,\ v_i = x\}$, where K is some finite subset of $\mathbb{Z}$. For any initial configuration $u \in \mathcal{A}^{\mathbb{Z}}$, using the ergodicity of P, we have: $\delta_u P^n(C) \longrightarrow \delta_{x^{\mathbb{Z}}}(C) = 1$. But $\delta_u P^n$ is a Dirac measure, so $\delta_u P^n(C)$ is equal to 0 or 1. Consequently, we have $\delta_u P^n(C) = 1$ for n large enough, that is, $\exists N \in \mathbb{N}, \forall n \geq N, \forall i \in K,\quad P^n(u)_i = x$.

In words, in any space-time diagram of P, any column becomes eventually equal to $xxx\cdots$. Using the terminology of Guillon & Richard [8], the DCA P has a *weakly nilpotent trace*. It is proved in [8] that the weak nilpotency of the trace implies the nilpotency of the DCA. (The result is proved for cellular automata on $\mathbb{Z}$ and left open in larger dimensions.) This completes the proof. ◀

Kari proved in [10] that the nilpotency of a DCA on $\mathbb{Z}$ is undecidable. (For DCA on $\mathbb{Z}^d$, $d \geq 2$, the proof appears in [4].) By coupling Kari's result with Theorem 3.3, we get:

▶ **Corollary 3.4.** *Consider a DCA P on the set of cells $\mathbb{Z}$. The ergodicity of P in undecidable.*

The undecidability of the ergodicity of a PCA was a known result, proved by Kurdyumov, see [17], see also Toom [15]. But the undecidability of the ergodicity of a DCA, which is a stronger result, was in fact mentioned as *Unsolved Problem 4.5* in [16].

Corollary 3.4 can also be obtained without Theorem 3.3, by directly adapting Kari's proof to show the undecidability of the ergodicity of the DCA associated with a NW-deterministic tile set.

4 Sampling the invariant measure of an ergodic PCA

Generally, the invariant measure(s) of a PCA cannot be described explicitly. Numerical simulations are consequently very useful to get an idea of the behavior of a PCA. Given an ergodic PCA, we propose a *perfect sampling* algorithm which generates configurations *exactly* according to the invariant measure.

A perfect sampling procedure for finite Markov chains has been proposed by Propp & Wilson [12] using a *coupling from the past* scheme. Perfect sampling procedures have been developed since in various contexts. Let us mention some related works. For more information see the annotated bibliography: *Perfectly Random Sampling with Markov Chains*, `http://dimacs.rutgers.edu/~dbwilson/exact.html/`.

The complexity of the algorithm depends on the number of all possible initial conditions, which is prohibitive for PCA. A first crucial observation already appears in [12]: for a monotone Markov chain, one has to consider only extremal initial conditions. To cope with more general situations, Huber [9] introduced the idea of a bounding chain for determining when coupling has occurred. The construction of these bounding chains is model-dependent and in general not straightforward. In the case of a Markov chain on a lattice, Bušić et al. [2] proposed an algorithm to construct the bounding chains.

Our contribution is to show that the bounding chain ideas can be given in a particularly simple and convenient form in the context of PCA via the introduction of the *envelope PCA*.

4.1 Basic coupling from the past for PCA

We present first the algorithm for a PCA on a finite set of cells, and then for an infinite set of cells.

Finite set of cells. Consider an ergodic PCA P on the alphabet $\mathcal{A}$ and on a finite set of cells E (for example $\mathbb{Z}_m = \mathbb{Z}/m\mathbb{Z}$). Let π be the invariant measure on $X = \mathcal{A}^E$. A *perfect sampling* procedure is a random algorithm which returns a state $x \in X$ with probability $\pi(x)$. Algorithm 1 is a presentation of the Propp & Wilson, or *coupling from the past (CFTP)*, perfect sampling procedure, written here in the context of PCA.

▶ **Proposition 4.1** ([12]). *If Algorithm 1 stops almost surely, then the PCA is ergodic and the output is distributed according to the invariant measure.*

Algorithm 1: Basic CFTP algorithm for a finite set of cells

Data: Update function $\phi : X \times [0,1]^E \to X$ of a PCA. Family $(r_k^{-n})_{(k,n)\in E\times\mathbb{N}}$ of i.i.d. r.v. uniform on $[0,1]$.

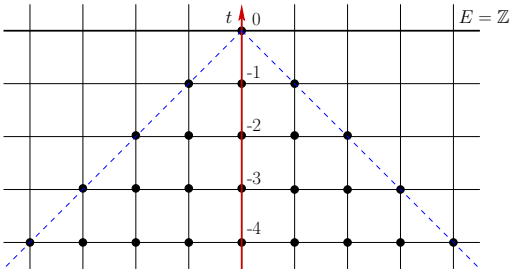
```
begin
    t = 1 ;
    repeat
        R_{-t} = X ;
        for j = -t to -1 do
            R_{j+1} = {φ(x, (r_i^j)_{i∈E}) ; x ∈ R_j}
        t = t + 1
    until |R_0| = 1 ;
    return the unique element of R_0
end
```

The proof is based on the following idea: if we had run the Markov chain from time $-\infty$ up to 0, then the result would obviously be equal to the output of the algorithm. But if we start from time $-\infty$, the Markov chain has reached equilibrium by time 0.

Infinite set of cells. Assume that the set of cells E is infinite. Then a PCA defines a Markov chain on the infinite state space $X = \mathcal{A}^E$, so the above procedure is not effective anymore. However, it is possible to use the locality of the updating rule of a PCA to still define a perfect sampling procedure. (This observation already appears in [1].)

Let P be an ergodic PCA P and denote by π its invariant distribution. In this context, a *perfect sampling* procedure is a random algorithm taking as input a finite subset K of E and returning a cylinder $x_K \in \mathcal{C}(K)$ with probability $\pi(x_K)$.

To get such a procedure, we use the following fact: if the PCA is run from time $-k$ onwards, then to compute the content of the cells in K at time 0, it is enough to consider the cells in the finite dependence cone of K. This is illustrated here for the set of cells $E = \mathbb{Z}$ and the neighborhood $V = \{-1, 0, 1\}$, with the choice $K = \{0\}$.



More formally, let V be the neighborhood of the PCA. Given a subset K of E, the *dependence cone* of K is the family $(V_{-t}(K))_{t\in\mathbb{N}}$ of subsets of E defined recursively by $V_0(K) = K$ and $V_{-t}(K) = V + V_{-t+1}(K)$. Let $\phi : X \times [0,1]^E \to X$ be an update function, for instance the one defined in (1). For a given subset K of E, we denote $\phi_{-t} : \mathcal{A}^{V_{-t}(K)} \times [0,1]^{V_{-t}(K)} \to \mathcal{A}^{V_{-t+1}(K)}$ the corresponding restriction of ϕ. With these notations, the algorithm now consists in setting at each step $R_{-t} = \mathcal{A}^{V_{-t}(K)}$ and computing $R_{j+1} = \{\phi_j(x, (r_i^j)_{i\in V_j(K)}) \,;\, x \in R_j\} \subset \mathcal{A}^{V_{j+1}(K)}$ for $j = -t$ to -1. This is done until we get $|R_0| = 1$.

Next proposition is an easy extension of Proposition 4.1.

▶ **Proposition 4.2.** *If the procedure stops almost surely, then the PCA is ergodic and the output is distributed according to the marginal of the invariant measure.*

4.2 Envelope probabilistic cellular automata (EPCA)

The CFTP algorithm is inefficient when the state space is large. This is the case for PCA: when E is finite, the set $\mathcal{A}^E$ is very large, and when E is infinite, it is the dependence cone described above which is very large. We cope with this difficulty by introducing the *envelope* PCA.

For simplicity, we assume that P is a PCA on the alphabet $\mathcal{A} = \{0, 1\}$ (as previously, the set of cells is denoted by E, the neighborhood by $V \subset E$ and the local function by f). Most of the results can be easily extended to the case of a general alphabet.

Definition of the EPCA. Let us introduce a new alphabet: $\mathcal{B} = \{\mathbf{0}, \mathbf{1}, ?\}$. A word on $\mathcal{B}$ is to be thought as a word on $\mathcal{A}$ in which the letters corresponding to some positions are not known, and are thus replaced by the symbol "?". Formally we identify $\mathcal{B}$ with $2^{\mathcal{A}} - \emptyset$ as follows: $\mathbf{0} = \{0\}$, $\mathbf{1} = \{1\}$, and $? = \{0, 1\}$. So each letter of $\mathcal{B}$ is a set of possible letters of $\mathcal{A}$. With this interpretation, we view a word on $\mathcal{B}$ as a set of words on $\mathcal{A}$. For instance, $?\mathbf{1}? = \{010, 011, 110, 111\}$.

We will associate to the PCA P a new PCA on the alphabet $\mathcal{B}$, that we call the *envelope probabilistic cellular automaton* of P.

▶ **Definition 4.3.** The *envelope probabilistic cellular automaton (EPCA)* of P, is the PCA $\mathrm{env}(P)$ of alphabet $\mathcal{B}$, defined on the set of cells E, with the same neighborhood V as for P, and a local function $\mathrm{env}(f) : \mathcal{B}^V \to \mathcal{M}(\mathcal{B})$ defined for each $y \in \mathcal{B}^V$ by

$$\mathrm{env}(f)(y)(\mathbf{0}) = \min_{x\in\mathcal{A}^V,\, x\in y} f(x)(0), \qquad \mathrm{env}(f)(y)(\mathbf{1}) = \min_{x\in\mathcal{A}^V,\, x\in y} f(x)(1)$$

$$\mathrm{env}(f)(y)(?) = 1 - \min_{x\in\mathcal{A}^V,\, x\in y} f(x)(0) - \min_{x\in\mathcal{A}^V,\, x\in y} f(x)(1).$$

Observe that $\mathrm{env}(P)$ acts like P on configurations which do not contain the letter "?". More precisely,

$$\forall y \in \mathcal{A}^V, \qquad \mathrm{env}(f)(y)(\mathbf{0}) = f(y)(0),\ \mathrm{env}(f)(y)(\mathbf{1}) = f(y)(1),\ \mathrm{env}(f)(y)(?) = 0\,. \tag{2}$$

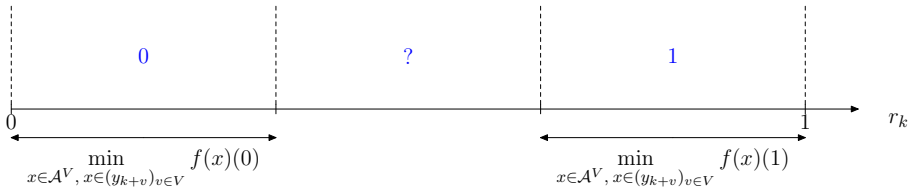
It implies next proposition. The converse statement is not true, see the counter-examples in Section 4.3.3.

▶ **Proposition 4.4.** *If the EPCA $\mathrm{env}(P)$ is ergodic then the PCA P is ergodic.*

Construction of an update function for the EPCA. Let us define the update function $\tilde{\phi} : \mathcal{B}^E \times [0,1]^E \to \mathcal{B}^E$ of the PCA $\mathrm{env}(P)$, by:

$$\tilde{\phi}(y,r)_k = \begin{cases} \mathbf{0} \text{ if } 0 \le r_k < \mathrm{env}(f)((y_{k+v})_{v\in V})(\mathbf{0}) \\ \mathbf{1} \text{ if } 1 - \mathrm{env}(f)((y_{k+v})_{v\in V})(\mathbf{1}) \le r_k \le 1 \\ ? \text{ otherwise.} \end{cases} \tag{3}$$

The value of $\tilde{\phi}(y,r)_k$ in function of r_k can be represented as follows:



Let ϕ be the natural update function for the PCA P defined in (1). Observe that $\tilde{\phi}$ coincides with ϕ on configurations which do not contain the letter "?". Furthermore, we have:

$$\forall r \in [0,1]^E,\ \forall x \in \mathcal{A}^E,\ \forall y \in \mathcal{B}^E, \qquad x \in y \implies \phi(x,r) \in \tilde{\phi}(y,r)\,. \tag{4}$$

4.3 Perfect sampling using EPCA

We propose two perfect sampling algorithms, for a finite and for an infinite number of cells. We show that in both cases, the algorithm stops almost surely if and only if the EPCA is ergodic. The ergodicity of the EPCA implies the ergodicity of the PCA but the converse is not true: we provide a counterexample for each case, finite and infinite.

We also give sufficient conditions of ergodicity of the EPCA.

4.3.1 Algorithms

The algorithm for a finite set of cells is given in Algorithm 2. For an infinite set of cells, we consider the dependence cone of a finite set of cells K (see Section 4.1).

Finite set of cells. The idea is to consider only one trajectory of the EPCA - the one that starts from the initial configuration $?^E$ (coding the set of all configurations of the PCA). The algorithm stops when at time 0, this trajectory hits the set $\mathcal{A}^E$.

Infinite set of cells. Once again, we consider only one trajectory of the EPCA: at each step , we set $c = ?^{V_{-t}(K)}$ and compute $c = \tilde{\phi}_j(c, (r_i^j)_{i\in V_j(K)}) \in \mathcal{B}^{V_{j+1}(K)}$ for $j = -t$ to -1. This is done until we get $c \in \mathcal{A}^K$.

Algorithm 2: Perfect sampling using the EPCA for a finite set of cells

```
Data: Update function φ̃. Family
      (r_k^{-n})_{(k,n)∈E×ℕ} of i.i.d. r.v.
      uniform on [0,1].
begin
    t = 1 ;
    repeat
        c = ?^E ;
        for j = −t to −1 do
            c = φ̃(c, (r_i^j)_{i∈E})
        t = t + 1
    until c ∈ A^E ;
    return c
end
```

▶ **Proposition 4.5.** *The algorithms above (finite and infinite cases) stop almost surely if and only if the EPCA is ergodic. In that case, the output of the algorithm is distributed according to the unique invariant measure of the PCA.*

Proof. The argument is the same in the finite and infinite cases. We give it for the finite case. Assume first that Algorithm 2 stops almost surely. By construction, it implies that for all μ_0, the measure $\mu_0\ \mathrm{env}(P)^n$ is asymptotically supported by $\mathcal{A}^E$. Therefore, we can strengthen the result in Proposition 4.4: the invariant measures of $\mathrm{env}(P)$ coincide with the invariant measures of P. In that case, $\mathrm{env}(P)$ is ergodic iff P is ergodic. Now recall that the update functions of P and $\mathrm{env}(P)$ satisfy (4). Thus, Algorithm 1 also stops almost surely. Furthermore, if we use the same samples $(r_k^{-n})_{(k,n)\in E\times\mathbb{N}}$, Algorithms 1 and 2 will have the same output. According to Proposition 4.1, this output is distributed according to the unique invariant measure of P. In particular, P is ergodic. So $\mathrm{env}(P)$ is ergodic.

Assume now that the EPCA is ergodic. The unique invariant measure π of $\mathrm{env}(P)$ has to be supported by $\mathcal{A}^E$. Also, by ergodicity, we have $\delta_{?^E}\ \mathrm{env}(P)^n \xrightarrow{w} \pi$. This means precisely that Algorithm 2 stops a.s. ◀

4.3.2 Criteria of ergodicity for the EPCA

▶ **Proposition 4.6.** *Let the set of cells be finite. The EPCA env(P) is ergodic if and only if we have env$(f)(?^V)(?) < 1$. This condition can also be written as:*

$$\min_{x\in\mathcal{A}^V} f(x)(0) + \min_{x\in\mathcal{A}^V} f(x)(1) > 0\,. \tag{5}$$

In particular, on a finite set of cells, if the PCA has positive rates (i.e. $\forall u \in \mathcal{A}^V, \forall a \in \mathcal{A},\ f(u)(a) > 0$), then Algorithm 2 stops a.s.

For an infinite set of cells the situation is more complex. Condition (5) is not sufficient to ensure the ergodicity of the EPCA. A counter-example is given in Section 4.3.3. First, we propose a rough sufficient condition of ergodicity

▶ **Proposition 4.7.** *Let $\alpha^* \in (0,1)$ be the critical probability of the percolation PCA with neighborhood V, see Examples 2.5 and 2.8. The EPCA env(P) is ergodic if*

$$\mathit{env}(f)(?^V)(?)\ <\ \alpha^* \tag{6}$$

and non-ergodic if

$$\min_{x \in \mathcal{B}^V - \mathcal{A}^V} env(f)(x)(?) \ > \ \alpha^*. \tag{7}$$

4.3.3 Counter-examples

Recall Proposition 4.4: [EPCA ergodic] $\implies$ [PCA ergodic]. We now show that the converse is not true.

Let us consider the PCA Majority defined at the beginning of Section 5. For n odd, the PCA is ergodic on the set of cells $\mathbb{Z}_n = \mathbb{Z}/n\mathbb{Z}$, by Proposition 5.1. However the associated EPCA satisfies $\mathrm{env}(f)(???) = \delta_?$. According to Proposition 4.6, the EPCA is not ergodic.

Consider the PCA of Example 2.4. This PCA has positive rates, in particular, it satisfies (5). So the EPCA is ergodic on a finite set of cells. Now let the set of cells be $\mathbb{Z}$.

The PCA is ergodic for $\varepsilon \in (0,1)$, see Example 2.7. Consider now the associated EPCA $\mathrm{env}(P)$. Assume for instance that $\varepsilon \in (0, 1/2)$. We have

$$\mathrm{env}(f)(u) = \begin{cases} f(u) & \text{if } u \in \{\mathbf{0}, \mathbf{1}\}^V \\ \varepsilon\delta_{\mathbf{0}} + \varepsilon\delta_{\mathbf{1}} + (1-2\varepsilon)\delta_? & \text{otherwise .} \end{cases}$$

By applying Proposition 4.7, $\mathrm{env}(P)$ is non-ergodic if $1 - 2\varepsilon > \alpha^*$.

5 The majority PCA: a case study

The *Majority* PCA is one of the simplest examples of PCA whose behaviour is not well understood. Therefore, it provides a good case study for our sampling algorithms.

Given $0 < \alpha < 1$, the PCA *Majority*(α), or simply *Majority*, is the PCA on the alphabet $\mathcal{A} = \{0,1\}$, with set of cells $E = \mathbb{Z}$ (or $\mathbb{Z}_n = \mathbb{Z}/n\mathbb{Z}$), neighborhood $V = \{-1, 0, 1\}$, and transition function

$$f(x,y,z) = \alpha\, \delta_{\mathrm{maj}(x,y,z)} + (1-\alpha)\, \delta_{1-y}\ ,$$

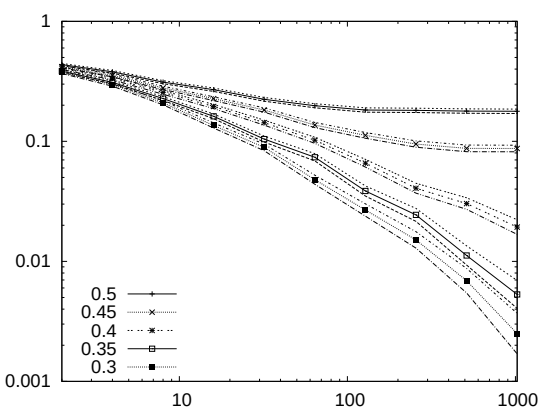
where $\mathrm{maj} : \mathcal{A}^3 \to \mathcal{A}$ is the *majority function*: the value of $\mathrm{maj}(x,y,z)$ is 0, resp. 1, if there are two or three 0's, resp 1's, in the sequence x, y, z. This PCA thus consists in choosing independently for each cell to apply rule 232 (with probability α) or to flip the value.

▶ **Proposition 5.1.** *Consider the Markov chain on the state space $\{0,1\}^{\mathbb{Z}_n}$ which is induced by the Majority PCA on set of cells $\mathbb{Z}_n$. The Markov chain has a unique invariant measure ν. If n is even then $\nu = (\delta_{(01)^{n/2}} + \delta_{(10)^{n/2}})/2$; if n is odd then ν is supported by $\{0,1\}^{\mathbb{Z}_n}$.*

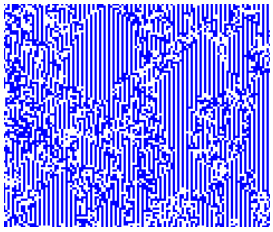
Let us consider now the PCA Majority on $\mathbb{Z}$. Let $x = (01)^{\mathbb{Z}} \in \{0,1\}^{\mathbb{Z}}$ be the configuration defined by: $\forall n \in \mathbb{Z}$, $x_{2n} = 0$, $x_{2n+1} = 1$. The configuration $(10)^{\mathbb{Z}}$ is defined similarly. The probability measure $\mu = (\delta_{(01)^{\mathbb{Z}}} + \delta_{(10)^{\mathbb{Z}}})/2$ is clearly an invariant measure for the PCA Majority. It can be viewed as the "limit" over n of the invariant measures of the PCA on $\mathbb{Z}_{2n}$. What about the "limits" of the invariant measures of the PCA on $\mathbb{Z}_{2n+1}$? Do they define other invariant measures for the PCA on $\mathbb{Z}$?

▶ **Conjecture 5.2.** *There exists $\alpha_c \in (0,1)$ such that* Majority(α) *has a unique invariant measure for $\alpha < \alpha_c$, and several invariant measures for $\alpha > \alpha_c$.*

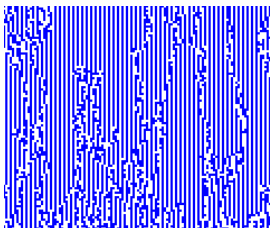
We propose a partial result relying on ideas of Regnault [13].



(a) The value of c_n as a function of n, for different α.



(b) $\alpha = 0.5$



(c) $\alpha = 0.3$

Figure 2 Experimental study of Majority(α) (the configurations at odd times only are represented on the space-time diagrams).

▶ **Proposition 5.3.** *Let p_c be the percolation threshold of directed bond-percolation in $\mathbb{N}^2$. If $\alpha \geq \sqrt[3]{1-(1-p_c)^4}$, then Majority($\alpha$) has several invariant measures. It is in particular the case if $\alpha \geq 0.996$.*

We also tried to come up with some numerical evidence. To study the PCA Majority experimentally, a first idea would be to consider the same PCA on the set of cells $\mathbb{Z}_n$, n odd, but this does not work well. First, computing exactly the invariant measure is impossible except for small n. Second the efficient perfect sampling is not available since the EPCA is not ergodic.

Instead, we used approximations of the PCA by a (non-homogeneous) PCA on the set of cells $D_n = \{-n, \ldots, n\}$, with random boundary conditions : at each step, the contents of cells $-n$ and n are updated using values of the cells $-(n+1)$ and $n+1$ chosen uniformly at random in $\{0, 1\}$. Again, computing exactly the invariant measure is impossible except for very small windows. But now, the EPCA is ergodic, and the perfect sampling algorithms become effective.

Let μ_n be the unique invariant measure for the set of cells D_n. Define

$$c_n = \mu_n\{x \in X \mid x_0 = x_1 = 0\} + \mu_n\{x \in X \mid x_0 = x_1 = 1\}\,.$$

One can prove that if $\limsup_n c_n > 0$, then there exists a non-trivial invariant measure for the PCA Majority on $\mathbb{Z}$ (this relies on the compactness of $\mathcal{M}(X)$).

The experimental results appear in Figure 2, with a logarithmic scale. We ran the sampling algorithms 10000 times, up to a window size of $n = 1024$. We show on the figure the confidence intervals calculated with Wilson score test at 95%.

It is reasonable to believe that the top two curves do not converge to 0 while the bottom three converge to 0. This is consistent with the visual impression of space-time diagrams. It reinforces Conjecture 5.2 with a possible phase transition between 0.4 and 0.45.

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References

1 J. van den Berg and J. E. Steif. On the existence and nonexistence of finitary codings for a class of random fields. *Ann. Probab.*, 27(3):1501–1522, 1999.
2 A. Bušić, B. Gaujal, and J.-M. Vincent. Perfect simulation and non-monotone markovian systems. In *Proceedings 3rd Int. Conf. Valuetools*. ICST, 2008.
3 P. Chassaing and J. Mairesse. A non-ergodic probabilistic cellular automaton with a unique invariant measure. arXiv:1009.0143, 2010.
4 K. Culik II, J. Pachl, and S. Yu. On the limit sets of cellular automata. *SIAM J. Comput.*, 18(4):831–842, 1989.
5 N. Fatès, D. Regnault, N. Schabanel, and E. Thierry. Asynchronous behavior of double-quiescent elementary cellular automata. In *LATIN 2006*, volume 3887 of *LNCS*, pages 455–466. Springer, 2006.
6 P. Gács. Reliable cellular automata with self-organization. *J. Statist. Phys.*, 103(1-2):45–267, 2001.
7 G. Grimmett. Percolation. Second edition. Springer-Verlag, Berlin, 1999.
8 P. Guillon and G. Richard. Nilpotency and limit sets of cellular automata. In *MFCS*, volume 5162 of *LNCS*, pages 375–386. Springer, 2008.
9 M. Huber. Perfect sampling using bounding chains. *Ann. Appl. Probab.*, 14(2):734–753, 2004.
10 J. Kari. The nilpotency problem of one-dimensional cellular automata. *SIAM J. Comput.*, 21(3):571–586, 1992.
11 Y. Le Borgne and J.-F. Marckert. Directed animals and gas models revisited. *Electron. J. Combin.*, 14(1):#R71, 2007.
12 J. Propp and D. Wilson. Exact sampling with coupled Markov chains. *Random Structures and Algorithms*, 9:223–252, 1996.
13 D. Regnault. Directed percolation arising in stochastic cellular automata analysis. In *MFCS 2008*, volume 5162 of *LNCS*, pages 563–574. Springer, Berlin, 2008.
14 N. Schabanel. Habilitation à Diriger des Recherches : Systèmes complexes & algorithmes. *Thesis.* LIAFA, CNRS and Université Paris Diderot - Paris 7, 2009.
15 A. Toom. Algorithmical unsolvability of the ergodicity problem for binary cellular automata. *Markov Process. Related Fields*, 6(4):569–577, 2000.
16 A. Toom. Contours, convex sets, and cellular automata. *IMPA Mathematical Publications.* IMPA, Rio de Janeiro, 2001.
17 A. Toom, N. Vasilyev, O. Stavskaya, L. Mityushin, G. Kurdyumov, and S. Pirogov. Discrete local Markov systems. In R. Dobrushin, V. Kryukov, and A. Toom, editors, *Stochastic cellular systems: ergodicity, memory, morphogenesis.* Manchester University Press, 1990.